A Study of Molecular Interactions Between the Associating Liquids and Their Binary Mixtures: A Dielectric and Volumetric Approach

Synopsis

Submitted to

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For the registration of the topic for
Doctor of Philosophy
in the subject of **PHYSICS**
(Faculty of Science)

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Abstract of proposed work plan/problem:

"A Study of Molecular Interactions Between the Associating Liquids and Their Binary: A Dielectric and Volumetric Approach"

1. Introduction :

A hydrogen bond is the basic of all the associating liquids. It is an attractive force between the hydrogen attached to an electronegative atom of one molecule and an electronegative atom of a different molecule. Usually an electronegative atom is Oxygen, Nitrogen or Fluorine which has the partial negative charge. The hydrogen then has the partial positive charge. The electronegative atom must have one or more unpaired electron pairs as in the case of oxygen and nitrogen, and has a negative partial charge. The hydrogen, which has partial positive charge tries to find another atom of oxygen or nitrogen with excess electrons to share and is attracted to partial negative charge. This forms the basis for hydrogen bond. Hydrogen bonding among the like and unlike molecules leads to two types molecular interactions. First, intramolecular interaction formed between the hydrogen atom and an atom of the electronegative element of the same molecule. Intramolecular hydrogen bond results in the cyclization of the molecules and prevents their association. Second, intermolecular interaction occurs when the hydrogen bonding is between H- atom of one molecule and atom of the electronegative of another molecule. For example hydrogen bond in alcohol and water. This results into association of molecules.

In order to study these molecular interactions among the associating liquids and their mixtures, Dielectric spectroscopy technique has proven its applicability for measurement of dielectric properties in a plethora of research papers [1-25].

It is planned to measure the complex permittivity spectra at various frequency range of these associating liquids and their binary mixtures. Further, these permittivity spectra will be used to investigate the dielectric and volumetric properties of binary mixtures of associating liquids in order to understand the significance of molecular interaction in them through hydrogen bonding.

2. Review of Literature and Development in the subject (Previous work done in the relevant area)

The TDR dielectric measurement system consists of a high frequency step generator which produces fast rising pulse of the order of picoseconds. A train of suitable fast rising pulses is applied to a coaxial transmission line of characteristic impedance of 50Ω. The literature survey shows that the experimental setup for time domain technique with various frequency ranges (upto 10GHz, 20GHz and 30GHz) has been successfully developed [26-29]. This technique is useful for the measurement of complex permittivity spectra of various polar, non-polar and binary mixtures of these systems. During last few decades this technique is extensively used to study structural behavior of associating liquids such as alcohols, diols, Polyhydric sugar alcohols, biomolecules, polymers, glycol ethers etc. at various frequency ranges [1-25]. These studies provide vital information on the molecular configuration of a system. High frequency molecular behavior of hydrogen bonded liquids provides information regarding their molecular interactions and dynamics and structural changes in the molecules, involved at the dipolar levels.

3. Objectives of Research/Proposed hypothesis:

- The precise measurement of complex permittivity of the associating liquids and their binary mixtures.
- Determine the static dielectric constant, relaxation time, high frequency dielectric permittivity by using suitable mathematical model from Havriliak–Negami (HN) equation (Eq.1) of these liquids.

$$\varepsilon^*(\omega) = \varepsilon_\infty + \frac{\varepsilon_0 - \varepsilon_\infty}{[1 + (j\omega\tau)^{1-\alpha}]^\beta} \qquad (1)$$

- To measure the refractive indices and densities of the associating liquids.
- To study molecular interactions in these systems using the dielectric and volumetric properties.

4. Methodology

A TDR technique has been successfully used to obtain information on the structural behavior and dynamic parameters of complex systems. The technique is used for the measurement of complex permittivity of polymers, bio-molecules at various frequency ranges. This may be anticipated to produce better dielectric relaxation parameters in this frequency range because the permittivity spectra are obtained by a single measurement. In the basic TDR system, a fast rising step voltage is propagated in an ideal coaxial line. The shape of step voltage remains unchanged as long as the propagation properties of the coaxial line remain the same.

The electrical and dielectric properties of these systems can be determined by using ‘capacitive measurement method’ at lower frequencies from few Hz to some MHz. The capacitances of the Liquid Dielectric Test Fixture with and without samples were measured

by using short compensation. The Test Fixture correction coefficient was also considered to cancel the stray capacitance during the determination dielectric constant values.

The refractive index of the liquid sample will be measured using Abbe's refractometer. The measurement of densities of the associating liquids can be done by using gravity bottle and precision weight machine.

5. Importance of study/society application:

The following scientists are doing research in this field at national/international level

- **International status:**

1. N Shiyanshiki, University of Tokyo, Tokyo, Japan
2. S Yagihara, University of Tokyo, Tokyo, Japan
3. S Sudo, Dept. of Physics, Tokyo City Univ. Tamazutsumi, Setagaya, Tokyo, Japan
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5. Udo Kaatze, Drittes Physikalisches Institut Georg-August-Universität Göttingen, Germany.

- **National Status:**

1. S C Mehrotra, Dr. BAMU, Aurangabad(MS).
2. R J Sengwa, JNV University, Jodhpur, Rajhsthan.
3. A C Kumbharkhane, SRTM University, Nanded (MS).
4. V A Rana, Gujrat University, Ahmedabad (Gujrat).

- **Significance of the study**

The dielectric properties of associating liquids are very remarkable. They typically display extremely high permittivity at low frequencies, their frequency dependence permits

identification and investigation of a number of completely different underlying mechanisms, and hence, dielectric studies of biomaterials have long been important in biophysics.

The natural observable fact involves the interaction between matter and energy. The nature and strength of molecular interactions in soft matter have been established as the cause for the behavioral change in chemical compounds. The extent of recognition of the most suitable and strongly proven structures involving certain chemical bonds and interactions are based on quite a number of qualitative and quantitative tests utilizing independent physical methods. IR, NMR, Ultrasonic and Dielectric Spectroscopy are a few among them. Dielectric relaxation studies will throw light on actual functioning of molecule. The dielectric spectroscopy method occupies a special place among the numerous modern methods used for physical and chemical analysis of material, because it enables investigation of dielectric relaxation processes in an extremely wide range of characteristics time.

6. Proposed work plan/Formulation and structure of study:

- **First Year:** To study the theoretical background of research problem and detail literature survey. Then choose the appropriate associating liquids for the dielectric measurements.

- **Second Year:** To study dielectric dispersion of these systems at different frequencies. To evaluate the dielectric properties such as static dielectric constant, relaxation time dielectric constant at high frequency for these systems. To measure the refractive indices and densities of these liquids.

- **Third Year:** Dielectric and volumetric information extracted from data analysis of these systems will be used further for interpretations of molecular behavior. These interpretations will be published by writing research papers or presenting the work in conference/seminars. Finally, write up thesis and complete the research work.

7. References:

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